Supplementary Information

(Appendices A, B, and C)

Optimal composition of chloride cells for osmoregulation in a randomly fluctuating environment

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Appendix A

Basic formulas and numerical analysis procedures

A.1 Derivation of basic formulas for dynamic programming

We consider the expected total load in the future if the current composition of chloride cell types is (x, y, z) and the current environment is i, where i indicates seawater ($i = s$) or freshwater ($i = f$). Given that we choose the optimal behavior in the future, the expected total load is represented as

$$V(x, y, z; i) = min\ E[\text{total load in the habitat}|\ (x, y, z), i]$$

The "min" symbol indicates that the fish choose the optimal behavior in the future. To derive a recursive formula, we decompose the expected future total load according to the events occurring in a short time interval Δt and the expected future total load after the interval:

$$V(x, y, z; s) = \Delta t \left[\frac{u_s - \theta}{x + z} + a_x x + a_y y + a_z z\right] + (1 - (p + \mu)\Delta t)V(x, y, z; s)$$

$$+p\Delta t \cdot min_{x\prime,y\prime,z\prime} \left[V(x', y', z'; f) + \tau(u_s - \theta)\left(\frac{1}{y+z} - \frac{1}{y\prime+z\prime}\right)\right] + O(\Delta t) \qquad \text{(A.1)}$$

In equation (A.1), the first term on the right-hand side is the workload plus maintenance cost experienced by the individual during a short period Δt. The first term in the braces is the daily stress experienced in seawater, which is due to the work of chloride cells coping with the difference of the osmotic pressure between inside and outside of the body. The other three terms are the daily maintenance costs, $a_x x + a_y y + a_z z$.

The second term on the right-hand side is the expected total cost if neither environmental change nor the end of the period occurs. p is the rate of environmental change from seawater to freshwater, and μ is the rate at which the individual leaves the focal habitat.

The third term on the right-hand side is the cost experienced if the environmental salinity changes. Note that environmental changes at rate p. Individuals might change the composition of three chloride cell types from (x, y, z) to (x', y', z'). The minimization operation in front of the braces indicates the optimal choice of the state after transition.

Within the braces are the sum of expected future total cost $V(x', y', z'; f)$ and the cost to be paid for the transition of cell composition, as explained in that last section.

By rearranging terms in equation (A.1) and calculating the limit of $\Delta t \to 0$, we can derive the following equation:

$$V(x, y, z; s) = \frac{1}{p+\mu}\left[\frac{u_s - \theta}{x+z} + a_x x + a_y y + a_z z\right] + \frac{p}{p+\mu} \cdot min_{x\prime, y\prime, z\prime}\left[V(x', y', z'; f) + \tau(\theta - u_f)\left(\frac{1}{y+z} - \frac{1}{y\prime + z\prime}\right)\right] \quad \text{(A.2a)}$$

for all (x, y, z) in Ω.

Similarly, for the environmental change from freshwater to seawater, we can derive the corresponding equation as follows:

$$V(x, y, z; f) = \frac{1}{q+\mu}\left[\frac{\theta - u_f}{y+z} + a_x x + a_y y + a_z z\right] + \frac{q}{q+\mu} \cdot min_{x\prime, y\prime, z\prime}\left[V(x', y', z'; s) + \tau(u_s - \theta)\left(\frac{1}{x+z} - \frac{1}{x\prime + z\prime}\right)\right] \quad \text{(A.2b)}$$

for all (x, y, z) in Ω.

Equations (A.2a) and (A.2b) can be intuitively understood as follows: For example, the first term on the right-hand side of equation (A.2a) is the sum of the workload and maintenance cost experienced by an individual in seawater while the current environment (seawater) lasts. The seawater environment will end either by environmental change at rate p or by the time the individual leaves the current habitat at rate μ. The term is the product of daily workload plus maintenance cost multiplied by the mean length of time of the period $1/(p+\mu)$. The second term of equation (A.2a) indicates the total workload after the next environmental change (which is from seawater to freshwater). This occurs with probability $p/(p+\mu)$. Then, the minimization operator indicates the optimal choice of cell composition made by the individual at the time of this environmental change to freshwater. Equation (A.2b) also has a similar interpretation.

Note that $V(x,y,z;s)$ for (x,y,z) in Ω includes $T(T+1)/2$ positive values in total. Combining $V(x,y,z;s)$ and $V(x,y,z;f)$ in Ω together, we have $T(T+1)$ numbers. They constitute a vector of $T(T+1)$-dimension. Equations (A.2a) and (A.2b) give a relationship to be satisfied by this vector.

A.2 Search for the future total cost

We search for the solution: $V(x,y,z;s)$ and $V(x,y,z;f)$ for all (x,y,z) in Ω that satisfy equations (4a) and (4b) in text. Note that they together include $T(T+1)$ numbers because Ω includes $T(T+1)/2$ elements. Hence, we search for a $T(T+1)$-dimensional vector that appears on both sides of the equations. Note that the same vector is included both on the left side and on the right side of the equations. We can solve this problem by the following sequential approximation method.

[1] We set $V(x,y,z;s)=V(x,y,z;f)=0$ for all (x,y,z) in Ω.

[2] Using these values in the right-hand side of equations (A.3a) and (A.3b), the left-hand sides give $V(x,y,z;s)$ and $V(x,y,z;f)$ in the next step. Note that we need to calculate all (x,y,z) included in Ω in each environment (s and f).

[3] Repeat the procedure in [2].

[4] After a number of iterations (say approximately 20), both $V(x,y,z;s)$ and $V(x,y,z;f)$ stop changing. Then, we regard them as the solution (i.e., stationary solution) of equations (A.3a) and (A.3b).

In this method, each element of the $T(T+1)$-dimensional vector, $V(x,y,z;s)$ and $V(x,y,z;f)$ in Ω, is an increasing function of the vector on the right-hand sides.

A.3 Search for the optimal cell composition

Suppose we have a pair of functions, $V(x,y,z;s)$ and $V(x,y,z;f)$, that satisfy both equations (4a) and (4b) in the text. Using these, we determine a pair of cell type compositions: (x_s,y_s,z_s) and (x_f,y_f,z_f) that are the optimal composition of chloride cells in the respective environment.

The optimal chloride cell composition in freshwater (x_f,y_f,z_f) is the solution that attains the minimum in equation (4a) in text. Even if we know the vector $V(x,y,z;f)$ for all (x,y,z) in Ω, we need to know y_s and z_s that are included in the braces. Additionally, the optimal chloride cell composition in seawater (x_s,y_s,z_s) is the solution that attains the minimum in equation (4b), which however includes y_f and z_f. Hence, the calculation of (x_f,y_f,z_f) requires knowledge of (x_s,y_s,z_s), and the calculation of (x_s,y_s,z_s) requires knowledge of (x_f,y_f,z_f). This problem can be solved by the sequential approximation method again.

We first choose arbitrary initial type compositions, (x_s, y_s, z_s) and (x_f, y_f, z_f), in seawater and freshwater environments, respectively. From these, we obtain the type compositions in the two environments in the next step: $(x_f, y_f, z_f)^{next}$ is the chloride cell composition that attains the minimization operation in equation (4a), given (x_s, y_s, z_s). Similarly, $(x_s, y_s, z_s)^{next}$ is the chloride cell composition that attains the minimization operation in equation (4b), given (x_f, y_f, z_f). If we repeat this iteration, we reach the situation in which (x_s, y_s, z_s) and (x_f, y_f, z_f) no longer change. Then, we can regard them as the optimal chloride cell composition in the two environments under stochastically fluctuating environments.

Appendix B

Here, we solve for the optimal chloride cell composition in seawater, (x_s, y_s, z_s). It is the one that achieves the minimum of equation (4a) under $x + y + z = T$, $x \geq 0$, $y \geq 0$, and $z \geq 0$. By eliminating z, this is rewritten as minimizing

$$\psi(x, y) = \frac{C}{T-y} + a_z T - (a_z - a_x)x - \left(a_z - a_y\right)y + \frac{F}{T-x} \qquad \text{(B.1)}$$

within a triangular region: $x + y \leq T$, $x \geq 0$, and $y \geq 0$. This attains the minimum at $(x, y) = (x_s, y_s)$. In equation (B.1), we denote $C = (1 - (p + \mu)\tau)(u_s - \theta)$ and $F = p\tau\left(\theta - u_f\right)$. $C > F$ holds because the period needed for new chloride cells to mature τ is much shorter than the mean lengths of two environments, $1/(p + \mu)$ and $1/(q + \mu)$.

We calculate the Hessian matrix of function $\psi(x, y)$. We have

$$\frac{\partial \psi}{\partial x} = \frac{F}{(T-x)^2} - (a_z - a_x),\ \frac{\partial \psi}{\partial y} = \frac{C}{(T-y)^2} - \left(a_z - a_y\right),$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2F}{(T-x)^3},\ \frac{\partial^2 \psi}{\partial x \partial y} = 0,\ \frac{\partial^2 \psi}{\partial y^2} = \frac{2C}{(T-y)^3} \qquad \text{(B.2)}$$

The Hessian matrix is positive definite (both eigenvalues are real and positive) at all (x, y) within the triangular region. Hence, if we find a local minimum of equation (B.1), it is also the global minimum.

B.1 Four phases for optimal chloride cell composition in seawater

In the following, we examine candidate solutions for a local minimum of $\psi(x, y)$. We examine four different cases, numbered as the fraction of generalist chloride cells z_s decreases.

Phase I All cells are generalists.

$x_s = 0,\ y_s = 0$, and $z_s = T$. This vertex solution is a local minimum if a small deviation would make $\psi(x, y)$ larger. This condition corresponds to the following:

$$\frac{\partial\psi}{\partial x} = \frac{F}{T^2} - (a_z - a_x) > 0 \text{ and } \frac{\partial\psi}{\partial y} = \frac{C}{T^2} - (a_z - a_y) > 0 \quad \text{(B.3)}$$

according to equation (B.2). If both of these hold, the solution $(x, y) = (0,0)$ is the global minimum. In contrast, if an opposite inequality holds for at least one of these two, it is not the minimum. Equation (B.3) becomes

$$a_z - a_x < \frac{p\tau(\theta - u_f)}{T^2} \text{ and } a_z - a_y < \frac{(1-(p+\mu)\tau)(\theta - u_f)}{T^2} \quad \text{(B.4)}$$

Because τ is small, the first inequality is stricter than the second inequality.

Phase II A mixture of generalist cells and specialist cells that are adapted to the current environment.

We consider, $x_s = \xi,\ z_s = T - \xi$. and $y_s = 0$, when ξ is a value between 0 and 1 ($0 < \xi < 1$). This includes specialist cells adapted to the current environment (seawater) but no specialists adapted to the future environment (freshwater). This solution is the local minimum if the following conditions are satisfied.

$$\frac{\partial\psi}{\partial x} = \frac{F}{(T-\xi)^2} - (a_z - a_x) = 0 \quad \text{(B.4a)}$$

$$\frac{\partial\psi}{\partial y} = \frac{C}{T^2} - (a_z - a_y) > 0 \quad \text{(B.4b)}$$

From equation (B.4a), we can determine the solution:

$$x_s = T - \sqrt{\frac{p\tau(\theta - u_f)}{a_z - a_x}},\ y_s = 0 \text{ and } z_s = \sqrt{\frac{p\tau(\theta - u_f)}{a_z - a_x}}. \quad \text{(B.5)}$$

if $a_z - a_x > \frac{p\tau(\theta - u_f)}{T^2}$ holds. If $a_z - a_x < \frac{p\tau(\theta - u_f)}{T^2}$ holds instead, then the edge solution equation (B.5) does not exist. If it exists, then it is the minimum when condition (B.4b) holds, which is rewritten as

$$a_z - a_y < \frac{(1-(p+\mu)\tau)(u_s-\theta)}{T^2}.$$

Phase III All three types exist with positive fractions.

$x_s = \eta > 0,\ y_s = \xi > 0$, and $z_s = T - \eta - \xi > 0$. From equation (B.2), we have

$$\frac{\partial\psi}{\partial x} = \frac{F}{(T-\eta)^2} - (a_z - a_x) = 0 \ \text{ and } \frac{\partial\psi}{\partial y} = \frac{C}{(T-\xi)^2} - \left(a_z - a_y\right) = 0$$

which leads to

$$x_s = T - \sqrt{\frac{p\tau(\theta-u_f)}{a_z-a_x}},\ y_s = T - \sqrt{\frac{(1-(p+\mu)\tau)(u_s-\theta)}{a_z-a_y}},$$

$$\text{and} \qquad z_s = \sqrt{\frac{p\tau(\theta-u_f)}{a_z-a_x}} + \sqrt{\frac{(1-(p+\mu)\tau)(u_s-\theta)}{a_z-a_y}} - T \tag{B.6}$$

We need to confirm that all of these are positive. If so, equation (B.6) is the stationary solution within the triangular region. It is the global optimum because the Hessian matrix is positive definite.

Phase IV Mixture of two specialist chloride cell types (no generalist cells)

If the cost of generalist cells is large, the optimal solution includes no generalist cells. Let η be a positive value intermediate between 0 and 1 ($0 < \eta < 1$).

$x_s = \eta,\ y_s = T - \eta$, and $z_s = 0$

Equation (B.1) becomes

$$\psi = \frac{C}{\eta} + a_z T - (a_z - a_x)\eta - \left(a_z - a_y\right)(T - \eta) + \frac{F}{T-\eta} \tag{B.7}$$

One necessary condition for this to be a local minimum is $d\psi/d\eta = 0$, which is rewritten as

$$-\frac{C}{\eta^2} + \left(a_x - a_y\right) + \frac{F}{(T-\eta)^2} = 0. \tag{B.8}$$

Equation (B.8) is the equation determining the mixture of two specialist chloride cells.

To confirm the optimality of this solution, which is located on an edge ($x + y = T$), we need to check that the value of ψ increases as we move inward along a line perpendicular to the edge, which leads to

$$\frac{\partial\psi}{\partial x} + \frac{\partial\psi}{\partial y} < 0$$

which becomes

$$a_z - \frac{a_x + a_y}{2} > \frac{1}{2}\left(\frac{F}{(T-\eta)^2} + \frac{C}{\eta^2}\right), \tag{B.9}$$

where η is the solution of equation (B.8). Equation (B.9) indicates that the excess cost of generalist chloride cells is sufficiently large.

We can construct a candidate of the optimal solution satisfying equation (B.9). We define a_{zc} as the solution where Phase III ends. It is the solution of the following equation.

$$\sqrt{\frac{p\tau(\theta - u_f)}{a_{zc} - a_x}} + \sqrt{\frac{(1-(p+\mu)\tau)(u_s - \theta)}{a_{zc} - a_y}} - T = 0 \tag{B.10}$$

We set the following:

$$x_s = T - \sqrt{\frac{p\tau(\theta - u_f)}{a_{zc} - a_x}} \text{ and } y_s = T - \sqrt{\frac{(1-(p+\mu)\tau)(u_s - \theta)}{a_{zc} - a_y}}. \tag{B.11}$$

We show this satisfies equation (B.8) as follows: First, we confirm $x_s + y_s = T$ from equation (B.6). By setting $\eta = T - y_s = \sqrt{\frac{(1-(p+\mu)\tau)(u_s - \theta)}{a_{zc} - a_y}}$ and $T - \eta = T - x_s = \sqrt{\frac{p\tau(\theta - u_f)}{a_{zc} - a_x}}$, we have

$$-\frac{C}{\eta^2} = -\frac{C(a_{zc} - a_y)}{(1-(p+\mu)\tau)(u_s - \theta)} \text{ and } \frac{F}{(T-\eta)^2} = \frac{F(a_{zc} - a_x)}{p\tau(\theta - u_f)}$$

The left-hand side of equation (B.8) is

$$-\frac{C}{\eta^2} + (a_x - a_y) + \frac{F}{(T-\eta)^2} = -\frac{C(a_{zc} - a_y)}{(1-(p+\mu)\tau)(u_s - \theta)} + a_x - a_y + \frac{F(a_{zc} - a_x)}{p\tau(\theta - u_f)}$$

$$= -(a_{zc} - a_y) + a_x - a_y + (a_{zc} - a_x) = 0.$$

Hence, equation (B.11) shows the optimal chloride cell composition in Phase IV. It is clear that the solution is one in Phase III, and hence, the optimal cell composition is continuously connected between Phases III and IV. Note that equation (B.11) is independent of the cost of the generalist chloride cell a_z, which is plausible because no generalist chloride cell is included in the solution equation (B.11).

When $a_x = a_y$ holds, the maintenance cost is the same between two specialized chloride cells, and (B.8) can be solved as follows:

From our assumption that τ is much shorter than the length of each environment or the period of staying in the habitat, we can safely assume $(2p+\mu)\tau < 1$. If so, we can derive

$$\eta = T\frac{\sqrt{p\tau}}{\sqrt{1-(p+\mu)\tau}+\sqrt{p\tau}}$$

Hence, the optimal chloride cell composition is as follows:

$$x_s = T\frac{\sqrt{p\tau}}{\sqrt{1-(p+\mu)\tau}+\sqrt{p\tau}},\ y_s = T\frac{\sqrt{1-(p+\mu)\tau}}{\sqrt{1-(p+\mu)\tau}+\sqrt{p\tau}},\ \text{and}\ z_s = 0. \qquad \text{(B.12)}$$

Because there exists only one local minimum (n.b., the Hessian matrix is positive definite), we always have one solution that belongs to either Phase I, Phase II, Phase III or Phase IV, and it is the global optimum.

B.2 Optimal composition of chloride cells in freshwater

We have a similar solution for the optimal composition of chloride cells in freshwater (x_f, y_f, z_f), which is the one achieving the minimum of equation (4b) in text.

$$\psi(x,y) = \frac{C\prime}{T-y} + a_z T - (a_z - a_x)x - (a_z - a_y)y + \frac{F\prime}{T-x} \qquad \text{(B.13)}$$

within a triangular region: $x + y \leq T$, $x \geq 0$, and $y \geq 0$. This attains the minimum at $(x, y) = (x_f, y_f)$. In equation (B.1), we denote $C' = (1 - (q + \mu)\tau)(\theta - u_f)$ and $F' = q\tau(u_s - \theta)$. The solution is of four types, Phase I, Phase II, Phase III and Phase IV, in a similar manner as for (x_s, y_s, z_s), explained above.

Because chloride cell compositions in seawater (x_s, y_s, z_s) and in freshwater (x_f, y_f, z_f) are determined separately, these two solutions can belong to different phases. We show several examples later (see text and Appendix C).

Appendix C

Parameter dependences

Here, we explain how the model's behavior changes depending on the parameters for several cases illustrated in figures.

Figure S1 illustrates the optimal number of chloride cells of three types. (a) In seawater. The horizontal axis is $a_z - a_x$, the excess maintenance cost for the generalist cell. (b) In freshwater. Horizontal axis is $a_z - a_y$. Four cases are indicated by Roman numbers (I, II, III, IV). $p = 0.1$ is much larger than $q = 0.01$.

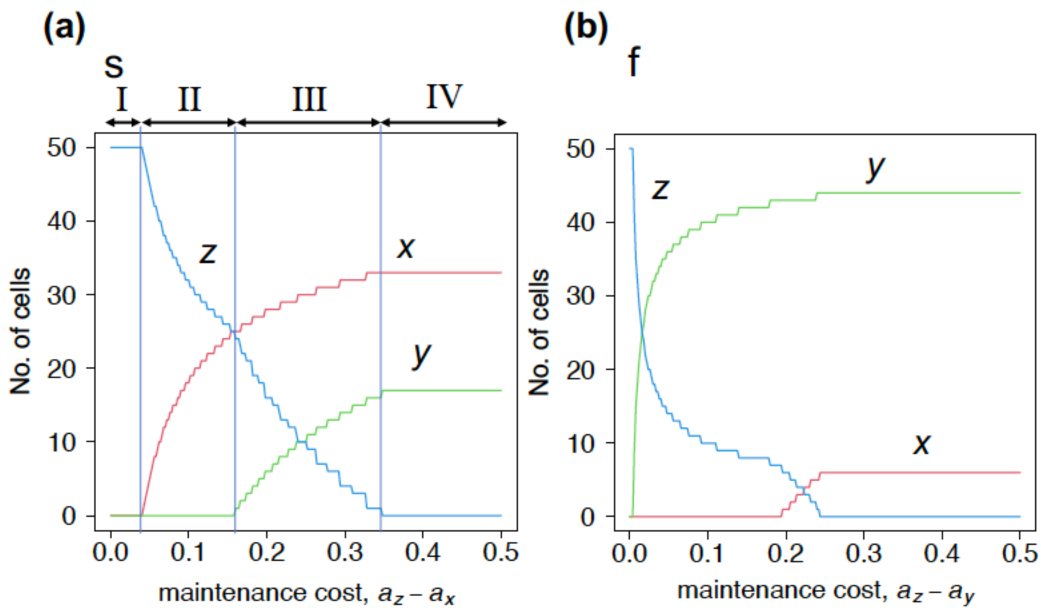

Figure S1 The optimal number of chloride cells of three types. (a) In seawater. Horizontal axis is $a_z - a_x$, the excess maintenance cost for the generalist cell. (b) In freshwater. Horizontal axis is $a_z - a_y$. The parameters are $p = 0.1$, $q = 0.01$, $\mu = 0.01$, $a_x = 0.01$, $a_y = 0.01$, $u_s = 1000$, $u_f = 0$, $\theta = 500$, $\tau = 2$, and $T = 50$.

Figure S2 illustrates the optimal number of chloride cells of three types. (a) In seawater. The horizontal axis is $a_z - a_x$, the excess maintenance cost for the generalist cell. (b) In freshwater. Horizontal axis is $a_z - a_y$. Four cases are indicated by Roman numbers (I, II, III, IV). $a_x = 0.01$ is smaller than $a_y = 0.05$. The excess maintenance cost of generalist cells is greater in seawater than in freshwater ($a_z - a_x > a_z - a_y$). The number of generalist cells z is smaller in seawater than in freshwater.

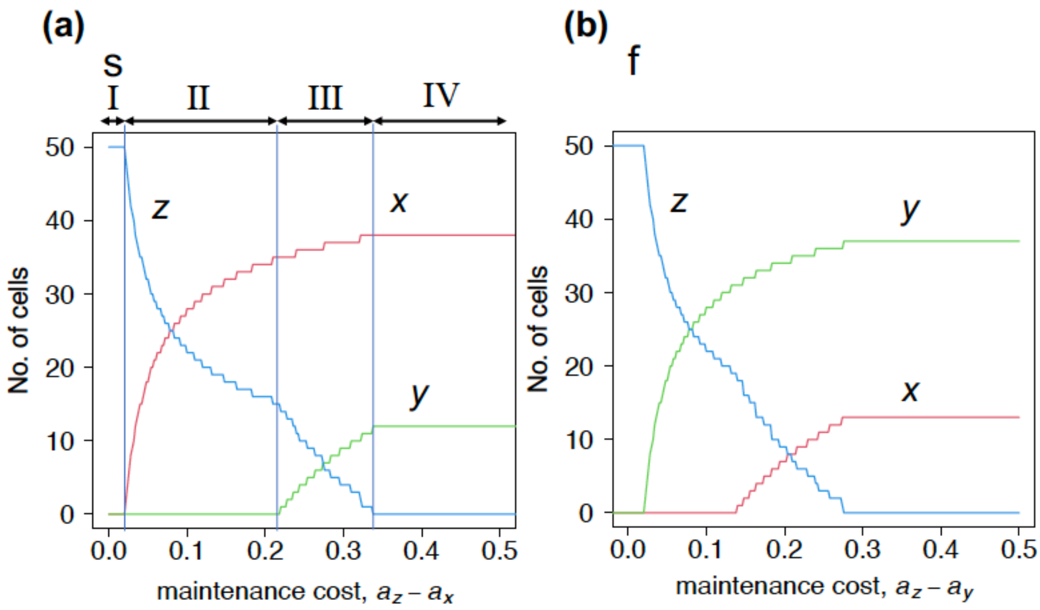

Figure S2 Optimal number of chloride cells of three types. (a) In seawater. The horizontal axis is $a_z - a_x$, the excess maintenance cost for the generalist cell. (b) In freshwater. Horizontal axis is $a_z - a_y$. The parameters are $a_x = 0.01$, $a_y = 0.05$, $\mu = 0.01$, $p = 0.05$, $q = 0.05$, $u_s = 1000$, $u_f = 0$, $\theta = 500$, $\tau = 2$, and $T = 50$.

Figure S3 illustrates the optimal number of chloride cells of three types in seawater. The horizontal axis is the osmotic pressure in the body, θ. Three parts have different time delays until new specialized cells mature: (a) $\tau = 0.5$; (b) $\tau = 2$; and (c) $\tau = 5$. The horizontal axis is θ, the osmotic pressure in the body. The four cases are indicated by Roman numbers (II, III, IV). The number of generalist chloride cells has a peak in the middle at a value of θ.

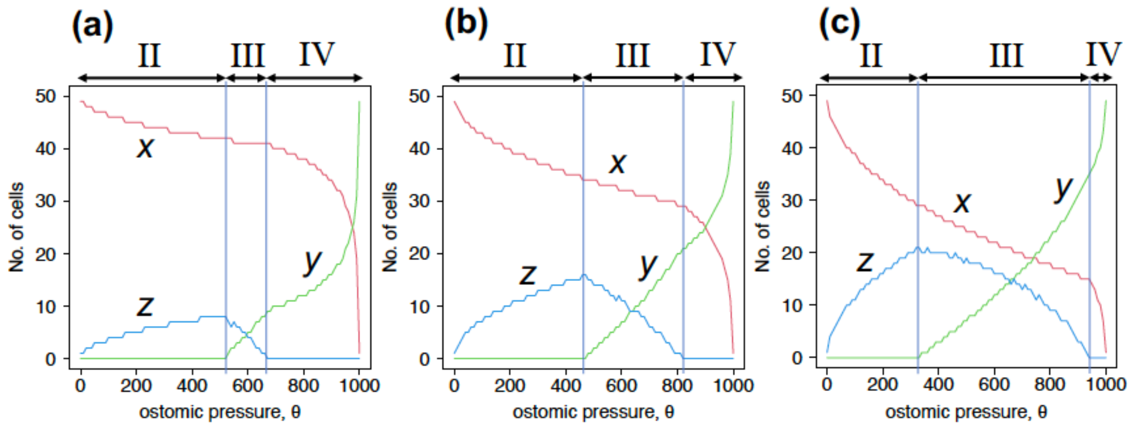

Figure S3 Optimal numbers of chloride cells of three types in seawater. Horizontal axis is θ. Three parts were subjected to different time delays until the new specialized cells matured. (a) $\tau = 0.5$; (b) $\tau = 2$; and (c) $\tau = 5$. Horizontal axis is θ, osmotic pressure of the body. Other parameters are $\mu = 0.01$, $p = 0.05$, $q = 0.05$, $a_x = 0.01$, $a_y = 0.01$, $u_s = 1000$, $u_f = 0$, $\tau = 2$, and $T = 50$.